Qualitative Analysis Report

Data Filename	TOX21_201890_TMS.D	**Sample Name**	NCGC Tox21_201890 from C13 SP109778
Position	61	**Instrument Name**	5975C_MR
User Name	Long	**Acq Method**	C1_28-0_2_520_mt384_sndv.M

User Chromatograms

Printed at: 10:22 AM on: 5/14/2014

Agilent Technologies
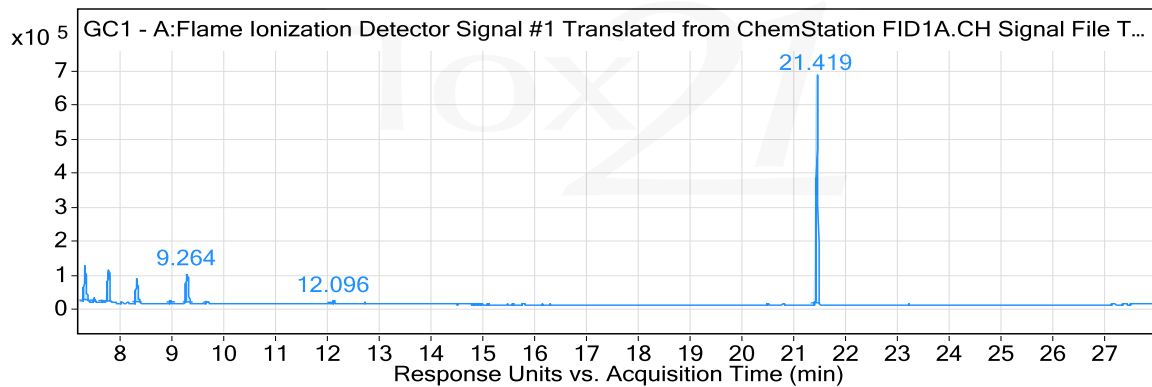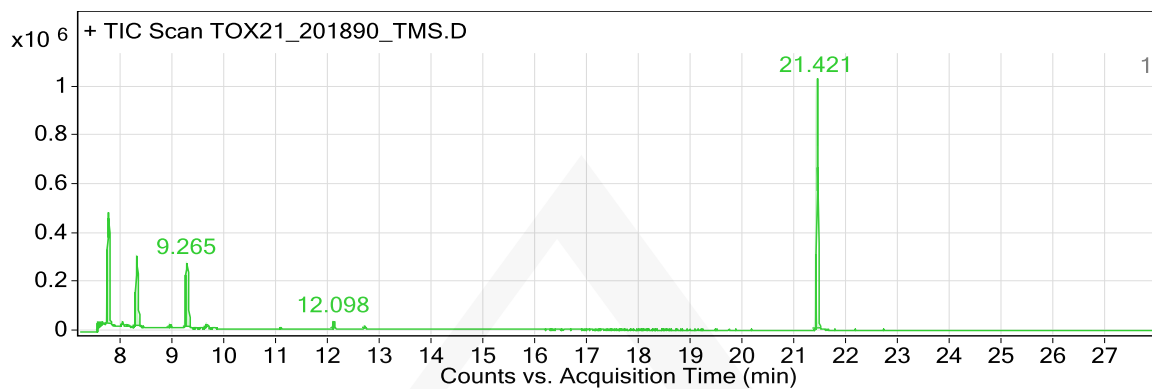
User Spectra

Spectrum Source
Peak (1) in "+ TIC Scan"

+ Scan (7.534-7.557 min, 5 Scans) TOX21_201890_TMS.D Subtract
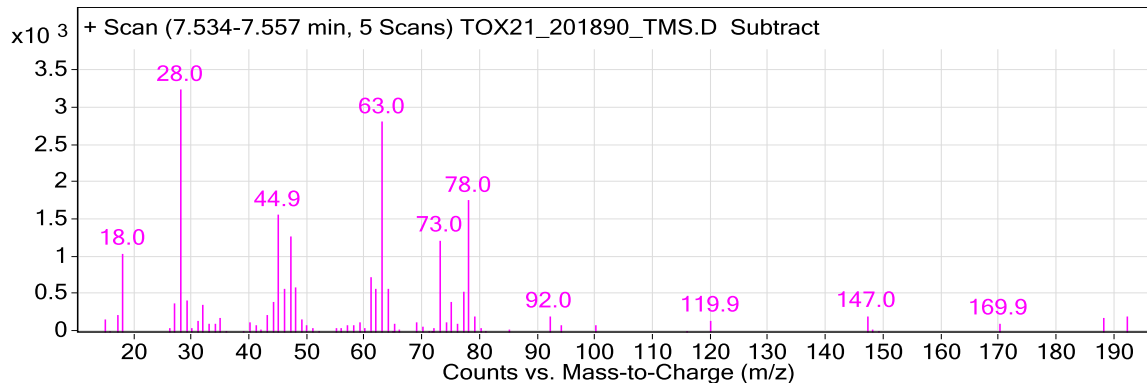
Spectrum Source
Peak (2) in "+ TIC Scan"

+ Scan (7.557-7.586 min, 6 Scans) TOX21_201890_TMS.D Subtract
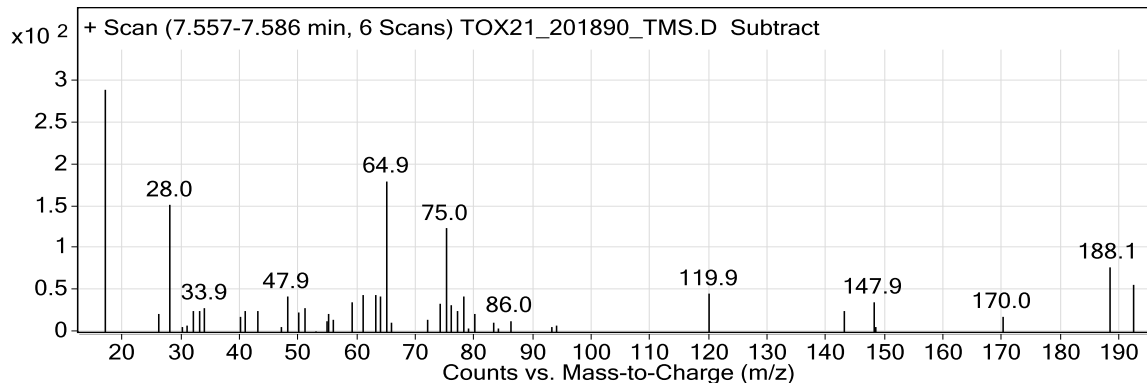
Spectrum Source
Peak (3) in "+ TIC Scan"

+ Scan (7.586-7.609 min, 5 Scans) TOX21_201890_TMS.D Subtract

Spectrum Source
Peak (4) in "+ TIC Scan"

+ Scan (7.609-7.644 min, 7 Scans) TOX21_201890_TMS.D Subtract

x10 2

Counts vs. Mass-to-Charge (m/z)

Peaks: 28.0, 45.0, 73.0, 63.0, 99.9, 85.2, 116.0, 133.0, 175.1, 192.1, 221.0
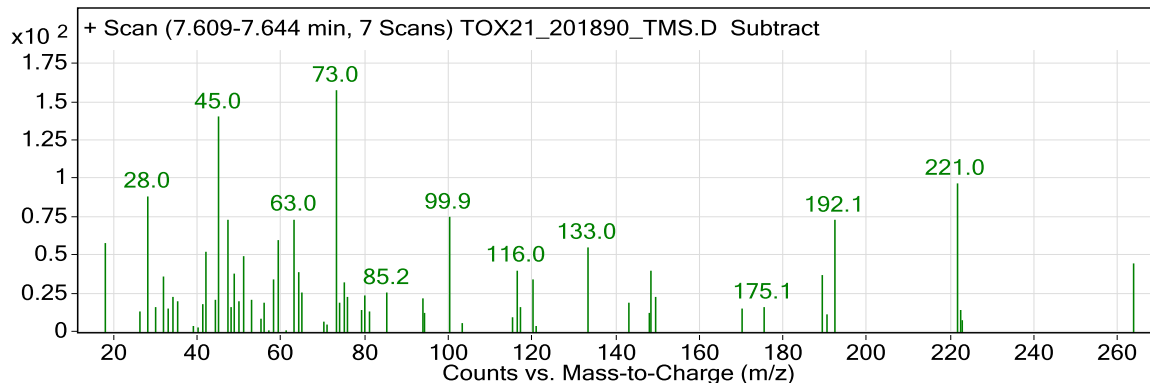
Spectrum Source
Peak (5) in "+ TIC Scan"

+ Scan (7.644-7.684 min, 8 Scans) TOX21_201890_TMS.D Subtract

x10 2

Counts vs. Mass-to-Charge (m/z)

Peaks: 18.0, 28.0, 43.9, 64.0, 76.0, 85.0, 92.0, 119.9, 143.0, 170.0, 192.0
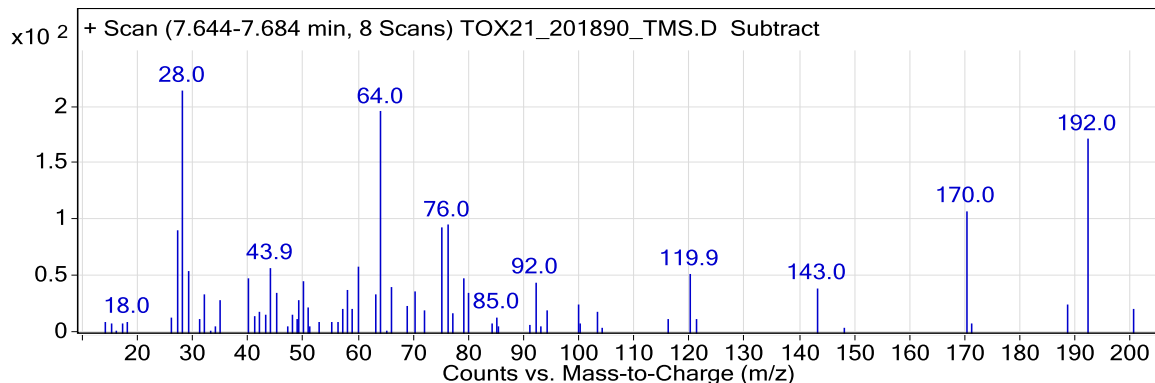
Spectrum Source
Peak (6) in "+ TIC Scan"

+ Scan (7.702-7.794 min, 17 Scans) TOX21_201890_TMS.D Subtract

x10 4

Counts vs. Mass-to-Charge (m/z)

Peaks: 15.0, 28.0, 45.0, 56.0, 61.0, 69.0, 78.0, 85.9, 97.0, 114.0, 126.0, 147.0, 173.0, 191.0
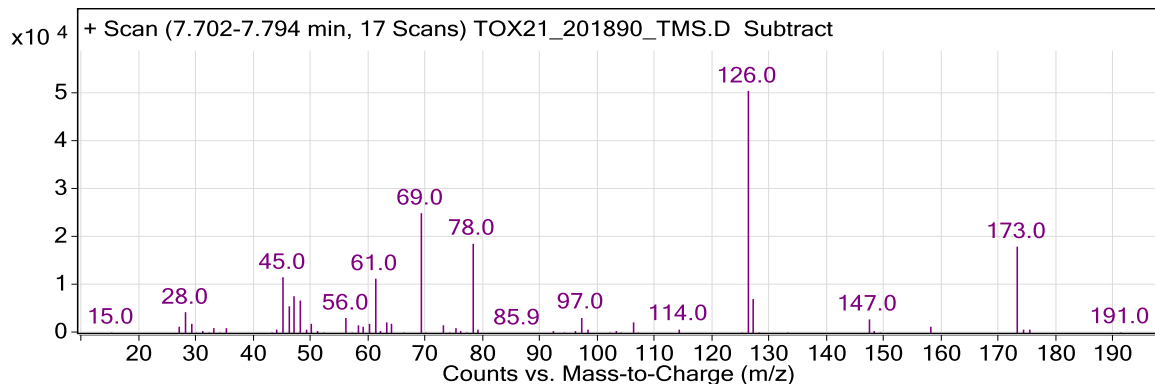
Qualitative Analysis Report

Spectrum Source
Peak (7) in "+ TIC Scan"

+ Scan (7.997-8.055 min, 11 Scans) TOX21_201890_TMS.D Subtract

x10 3

| m/z peaks labeled: |
28.0, 44.0, 56.0, 69.0, 78.0, 93.9, 113.9, 126.0, 141.0, 154.9, 170.0, 187.9

Counts vs. Mass-to-Charge (m/z)
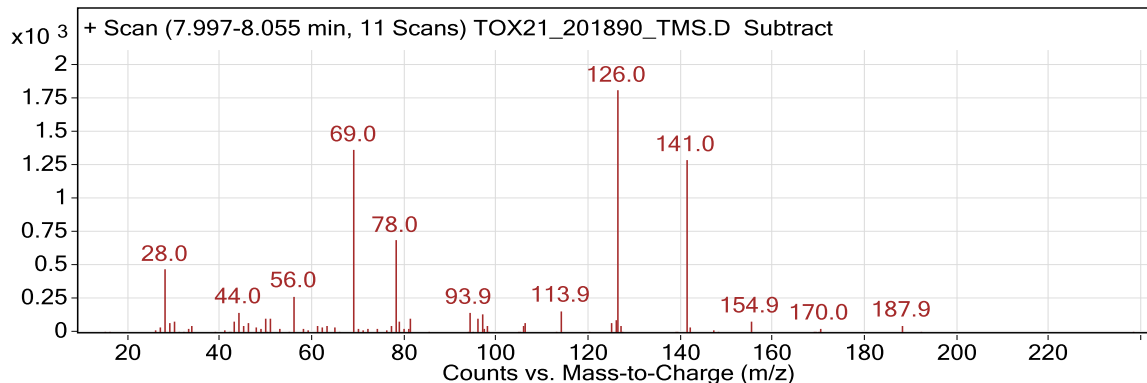
Spectrum Source
Peak (8) in "+ TIC Scan"

+ Scan (8.089-8.170 min, 15 Scans) TOX21_201890_TMS.D Subtract

x10 2

m/z peaks labeled: 18.0, 32.0, 44.9, 60.9, 75.0, 85.0, 100.9, 119.9, 129.0, 143.0, 157.0, 172.1

Counts vs. Mass-to-Charge (m/z)
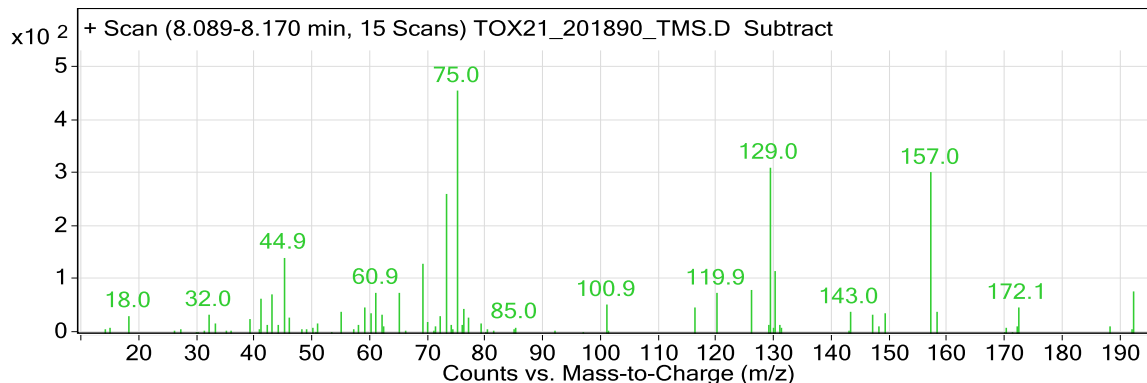
Spectrum Source
Peak (9) in "+ TIC Scan"

+ Scan (8.257-8.361 min, 19 Scans) TOX21_201890_TMS.D Subtract

x10 4

m/z peaks labeled: 27.0, 45.0, 61.0, 73.0, 90.9, 100.0, 120.0, 149.0, 169.0, 198.0, 216.0

Counts vs. Mass-to-Charge (m/z)

Spectrum Source
Peak (10) in "+ TIC Scan"

+ Scan (8.899-8.986 min, 16 Scans) TOX21_201890_TMS.D Subtract

x10 3

Peaks: 15.0, 29.0, 45.0, 58.9, 75.0, 84.9, 99.0, 111.0, 127.0, 142.0, 155.0, 170.1, 188.0

Counts vs. Mass-to-Charge (m/z)
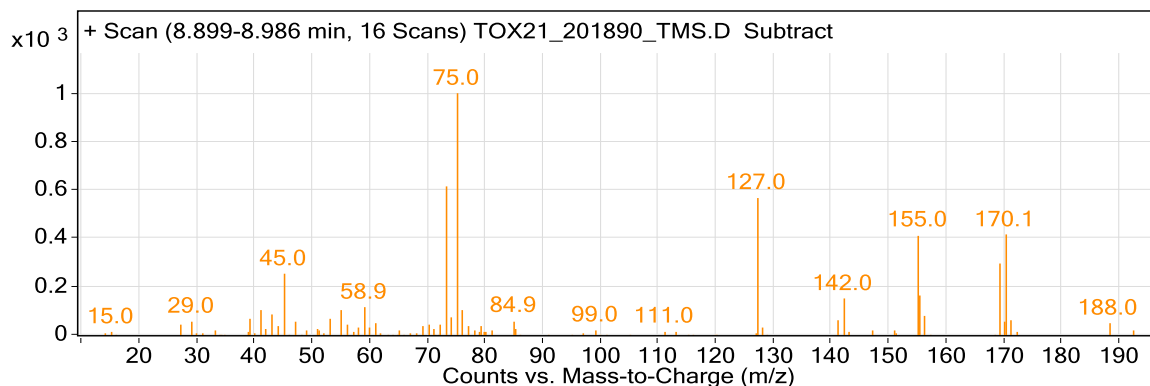
Spectrum Source
Peak (11) in "+ TIC Scan"

+ Scan (9.218-9.322 min, 19 Scans) TOX21_201890_TMS.D Subtract

x10 4

Peaks: 29.0, 45.0, 57.0, 64.9, 73.0, 93.0, 112.9, 128.9, 151.0, 169.9, 185.0

Counts vs. Mass-to-Charge (m/z)
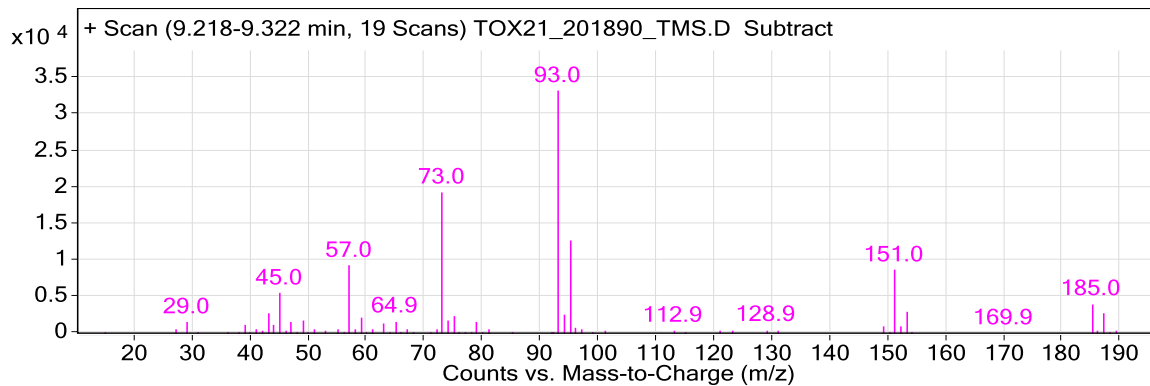
Spectrum Source
Peak (12) in "+ TIC Scan"

+ Scan (9.611-9.692 min, 15 Scans) TOX21_201890_TMS.D Subtract

x10 3

Peaks: 15.0, 28.9, 45.0, 58.0, 73.0, 87.9, 105.0, 120.0, 135.0, 150.1, 163.0, 188.1

Counts vs. Mass-to-Charge (m/z)

Spectrum Source
Peak (13) in "+ TIC Scan"

+ Scan (12.064-12.145 min, 15 Scans) TOX21_201890_TMS.D Subtract

x10 3

```
6
5        61.0
4
3
2
1    27.0  42.0      68.9    87.9       115.9      147.0          185.0
0
   20   40   60   80  100  120  140  160  180  200  220
        Counts vs. Mass-to-Charge (m/z)
```
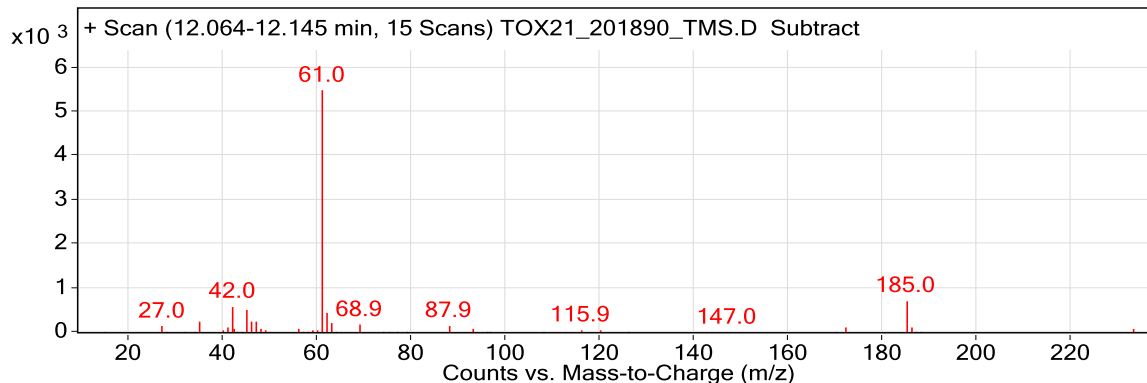
Spectrum Source
Peak (14) in "+ TIC Scan"

+ Scan (12.666-12.735 min, 13 Scans) TOX21_201890_TMS.D Subtract

x10 3

```
1.4                         104.0
1.2
1
0.8           62.0
0.6
0.4      47.0        88.9
0.2  28.0      68.9           125.8   146.9    170.0
0
   20  30  40  50  60  70  80  90  100 110 120 130 140 150 160 170 180 190
        Counts vs. Mass-to-Charge (m/z)
```
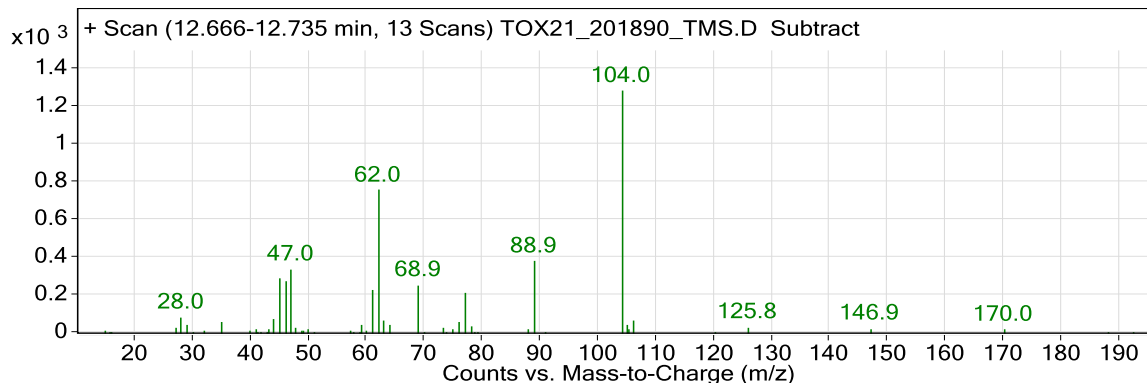
Spectrum Source
Peak (15) in "+ TIC Scan"

+ Scan (21.391-21.461 min, 13 Scans) TOX21_201890_TMS.D Subtract

x10 4

```
5                    75.0                                    313.3
4
3
2    43.1       103.0
1  29.0           143.0  171.1  199.1  227.2  255.1   297.2
0
   20  40  60  80  100 120 140 160 180 200 220 240 260 280 300 320
        Counts vs. Mass-to-Charge (m/z)
```

--- End Of Report ---